



15  
- 1. 12

## 1. Introduction

The Grant commenced on 1st June, 1983, initially for twelve months, but was extended for a further year to 31st May, 1985. The research, to be carried out at the University of Southampton, was to study turbulent transport in confined turbulent flames. Of special interest was the process of turbulent transport driven by a pressure gradient<sup>(1, 2)</sup>. The experimental programme was to involve the simultaneous use of Laser Doppler Anemometry and elastic (Mie) scattering from added seed particles to evaluate turbulent mass transport fluxes in the flame. A parallel theoretical study was to improve models of turbulent transport and hence to identify a suitable model for combustor flow field calculations.

However, the Grant was terminated, at the request of the University, with effect from 30th November, 1984. There were two reasons for this. The first was the long term illness and eventual resignation of the Research Assistant who had been appointed to carry out the experimental research. As a consequence of his absence essentially no progress was made in the experimental programme. The second reason was the departure of the Principal Investigator to take up an appointment at the University of Cambridge.

This Final Report is divided into three parts. The first deals briefly with the abortive experimental programme, while the second is concerned with theoretical model development where good progress was made. The third part of the report briefly discusses the question of models for combustor flowfield calculations.

## 2. Experiments

The experimental rig was a small ducted burner with a rectangular cross section incorporating four schlieren quality vitreous fused silica windows and supplied with premixed propane and air at velocities up to 20 m/s. The flow was uniformly seeded with  $T_1O_2$  particles which permitted simultaneous measurements to be made of gas density and axial flow velocity. The rig and experimental techniques have been described elsewhere<sup>(2)</sup>.

Although the Research Assistant learned to use these techniques and successfully reproduced some earlier published data, no new data of publishable quality was obtained. The reason for this failure was the long term illness and eventual resignation of the Research Assistant.

Experimental data obtained by these methods is described in earlier publications<sup>(2, 3)</sup>.

### 3. Theoretical Work

The objective of the theoretical programme was the exploration of theoretical models suitable for prediction of dump combustor flowfields. The starting point of this work was the model of premixed turbulent combustion developed by the Principal Investigator in collaboration with Professor P. A. Libby of University of California, San Diego and Professor J. B. Moss of Cranfield Institute of Technology<sup>(1, 4)</sup>.

Important progress was made in two areas during the period of the grant as described below.

#### 3.1 Scales of Scalar Field

Central features of the model of premixed turbulent combustion<sup>(1, 4)</sup> which forms the subject of this research are (i) the description of the thermochemistry in terms of a progress variable  $c$  which may be defined as a normalised product species concentration and (ii) consideration of a combustion regime in which the turbulent flame consists of thin moving interfaces at the boundaries between packets of unburned and fully burned gas. The combustion reactions then occur only within these interfaces. In this combustion regime the time average heat release rate is controlled by the length or time scales which determine the interface structure and its frequency of occurrence.

The instantaneous equation for the progress variable  $c$  is written<sup>(5)</sup>

$$\frac{\partial}{\partial t}(\rho c) + \frac{\partial}{\partial x_k} (\rho u_k c) = (\rho D_m) \frac{\partial^2 c}{\partial x_k^2} + w \quad (1)$$

where  $w$  is the chemical source term and subscript  $m$  represents a mean value. For statistically stationary conditions the mean of this equation at high Reynolds numbers where molecular transport may be neglected is

$$\frac{\partial}{\partial x_k} (\overline{\rho u_k c}) = \overline{w} \quad (2)$$

where  $\overline{w}$  is the time average of the source term  $w$ . Our objective is to derive an expression for  $\overline{w}$ .

Accession For	
NTIS CRA&I	<input checked="" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By _____	
Distribution/ _____	
Availability Codes	
Dist	Avail and/or Special
A-1	



We write<sup>(5)</sup>

$$\bar{w}(\underline{x}) = w_F(\underline{x}) v(\underline{x}) \quad (3)$$

where  $v(\underline{x})$  is the frequency at which flamelet interfaces cross location  $\underline{x}$  and

$$w_F = \langle \int_F w dt \rangle \quad (4)$$

is the chemical reaction occurring per crossing, where subscript F indicates integration through a flamelet interface and the triangular brackets denote a time average.

The analysis<sup>(5)</sup> may be divided into three parts. In the first part it is noted that, if the flamelet interfaces are thin,  $c(\underline{x}, t)$  at a fixed point  $\underline{x}$  is a square wave time series between  $c = 0$  and  $c = 1$ . This is modelled as a random telegraph signal, leading to the result that its autocovariance is<sup>(5)</sup>

$$P_{11}(\underline{x}, \hat{\tau}) \equiv \langle c(\underline{x}, t) c(\underline{x}, t + \hat{\tau}) \rangle = \bar{c}(1 - \bar{c}) \exp\left[-\frac{v\hat{\tau}}{2c(1-c)}\right] + \bar{c}^2 \quad (5)$$

The crossing frequency  $v$  is determined as

$$v = 2\bar{c}(1-\bar{c})/\hat{T} \quad (6)$$

where  $\hat{T}$  is an integral time scale:

$$T = \int_0^\infty \frac{P_{11} - \bar{c}^2}{\bar{c}(1-\bar{c})} d\hat{\tau} \quad (7)$$

A second stage of the analysis<sup>(5)</sup> is the formulation of a balance equation for  $T$ . This is done by writing Equation (1) at a location  $\underline{x}_1$  and time  $t_1$  and multiplying it by  $c$  evaluated at location  $\underline{x}_2$  and time  $t_2$ . Averaging then leads to a general two-point two-time covariance balance equation. The equation is specialized to one point and two times when it becomes a balance equation for the quantity  $P_{11}$  defined in Equation (5). Closure assumptions are made and the equation is integrated in  $\hat{\tau}$  to give the required balance equation for  $\hat{T}(\underline{x})$ . The balance equation shows that, with the modelling assumptions already introduced,  $\hat{T}$  is a constant.

Main features of the above analysis have been confirmed experimentally as reported in the original publication and since verified elsewhere<sup>(6, 7)</sup>.

The last part of the analysis is to model the chemical term  $w_F$  which appears in (3). This is represented<sup>(5)</sup> as

$$w_F = \frac{\rho_r S_L}{\bar{u} \cos \bar{\theta}} \quad (8)$$

where  $\rho_r$  is the density of unburned mixture,  $S_L$  is the laminar burning velocity of that mixture,  $\bar{u}$  is the Favre mean flow velocity, and  $\bar{\theta}$  is the average angle between  $\bar{u}$  and the direction normal to a flamelet. More recently<sup>(6)</sup>, Equation (8) has been replaced by an expression, based on an ensemble of strained laminar flamelets, which permits detailed chemical kinetics to be included.

An analysis of scalar length scales in premixed turbulent flames has also been reported<sup>(9)</sup>.

The advantages of the models described here, in comparison with earlier models, are that steps in the analysis can be tested experimentally and that detailed chemical kinetics of arbitrary complexity can be incorporated<sup>(8)</sup>.

### 3.2 Generalised Model for Turbulent Transport Fluxes

The model considered here<sup>(4)</sup> is what is known as a second order closure model in which a separate balance equation is formulated and solved for each second order covariance term such as a Reynolds stress component  $\bar{u}_j \bar{u}_k$  or a mass flux component  $\rho \bar{u}_j \bar{c}$ . It is necessary to go to this level of sophistication because the pressure gradient transport terms, which form a major focus of the work, appear here.

Previous work<sup>(1, 4)</sup> concentrated on planar one-dimensional turbulent flames separating regions of uniform flow in unburned and fully burned gases. Thus problems of modelling nonuniform turbulent flowfields in these unburned and fully burned regions were avoided.

The work reported here<sup>(10)</sup> proposes a general three dimensional set of second order closure equations. Unlike the equations used previously<sup>(1, 4)</sup> this set goes over properly to second order equations in the constant density low Mach number flows upstream and downstream of the turbulent flame.

A feature of second order closure models is that third order covariance terms appear and must be represented in terms of second order quantities. In the present work this is facilitated by the introduction of conditional velocities and turbulence quantities in reactant and product packets.

Thus for example<sup>(1)</sup>

$$\frac{\rho u_i'' u_j'' c''}{\bar{\rho}} / \bar{\rho} = \tilde{c} (1-\tilde{c}) \left[ \frac{(1-2c)(\bar{u}_{ip} - \bar{u}_{ir})}{\bar{\rho} \tilde{c}(1-c)} + \frac{(\bar{u}_{jp} - \bar{u}_{jr})}{\bar{\rho} \tilde{c}(1-c)} \right] + \frac{\bar{u}_i' u_{jp}'}{\bar{\rho}} - \frac{\bar{u}_i' u_{jr}'}{\bar{\rho}} \quad (9)$$

where the flamelet interfaces are thin. Here subscripts r and p refer to conditional quantities in reactants and products, respectively, so that for example  $\bar{u}_{ip} = \bar{c} u_i$ .

The model derived<sup>(10)</sup> from these considerations is

$$\frac{\rho u_i'' u_j'' c''}{\bar{\rho} \tilde{c}(1-\tilde{c})} = (1-2\tilde{c}) \frac{\rho u_i'' c''}{\bar{\rho} \tilde{c}(1-c)} \frac{\rho u_j'' c''}{\bar{\rho} \tilde{c}(1-c)} + g_{ij} \frac{\rho u_i'' u_j''}{\bar{\rho}} \quad (10)$$

$$\begin{aligned} \frac{\rho u_i'' u_j'' u_m''}{\bar{\rho}} &= - H_{ijm} + \tilde{c}(1-\tilde{c}) \left[ (1-2c) \frac{\rho u_i'' c''}{\bar{\rho} \tilde{c}(1-c)} \frac{\rho u_j'' c''}{\bar{\rho} \tilde{c}(1-c)} + g_{ij} \frac{\rho u_i'' u_j''}{\bar{\rho}} \right. \\ &\quad \left. + g_{im} \frac{\rho u_i'' u_m''}{\bar{\rho}} \frac{\rho u_j'' c''}{\bar{\rho} \tilde{c}(1-c)} + g_{jm} \frac{\rho u_j'' u_m''}{\bar{\rho}} \frac{\rho u_i'' c''}{\bar{\rho} \tilde{c}(1-c)} \right. \\ &\quad \left. + g_{im} \frac{\rho u_i'' u_m''}{\bar{\rho}} \frac{\rho u_j'' c''}{\bar{\rho} \tilde{c}(1-c)} \right] \end{aligned} \quad (11)$$

where

$$H_{ijm} = c_s \frac{\tilde{k}}{\tilde{c}} \frac{\rho u_k'' u_m''}{\bar{\rho}} \frac{\partial}{\partial x_k} \left( \frac{\rho u_i'' u_j''}{\bar{\rho}} \right)$$

$$g_{ij} = (1 - K_{ij1})c + (K_{ijo} - 1)(1-\tilde{c})$$

and  $c_s$ ,  $K_{ijo}$  and  $K_{ij1}$  are constants;  $\tilde{k}$  and  $\tilde{c}$  are the turbulence kinetic energy and dissipation function respectively.

Modelling of other terms in the second order balance equations has been discussed elsewhere<sup>(10)</sup>. The resulting set of modelled balance equations has been solved for a simple one dimensional flow<sup>(11)</sup> with satisfactory results.

4. Recommendations and Conclusions

A major objective of the research programme was to propose a theoretical model for premixed turbulent combustion which would be suitable for use in dump combustor flowfields. Processes of transport<sup>(1)</sup> and turbulence production<sup>(4)</sup> due to pressure gradients were to be taken into account. This objective has been met. The transport model recommended<sup>(10)</sup> is that described above in Section 3.2. The turbulent chemistry model should be that outlined in Section 3.1 as modified in a recent publication<sup>(8)</sup>. The modification permits the inclusion of detailed chemical kinetic mechanisms of arbitrary complexity through the introduction of an ensemble of strained laminar flamelets.

The experimental objectives of the programme were not achieved. This was a severe disappointment and the need for such experiments remains although some of the gaps in the experimental picture have since been filled, for example in Refs. (6, 7, 12, 13).

Notation

c	progress variable
$c_*$	constant, see Eq. (11)
D	diffusion coefficient
$\epsilon_{ij}$	see Eq. (10)
$H_{ijm}$	see Eq. (11)
$\tilde{k}$	Favre mean turbulence kinetic energy
$K_{ijo}$	constant, see Eq. (10)
$K_{ij1}$	constant, see Eq. (10)
$P_{11}$	autocovariance, see Eq. (5)
t	time
$s_L$	laminar burning velocity
$\hat{T}$	integral time scale, see Eq. (7)
$u_i$	i-th velocity component
w	chemical source term in Eq. (1)
$w_F$	see Eq. (3)
$x_k$	spatial coordinate
$\tilde{\epsilon}$	Favre mean viscous dissipation
$\bar{\theta}$	mean flame angle, see Eq. (8)
v	flamelet crossing frequency
$\rho$	density
$\tau$	time delay

Subscripts

i,j,k,m	spatial coordinates
p	products
r	reactants

Other

( )	mean value
( )'	Favre mean value
( )''	Favre fluctuation

References

1. P. A. Libby, K. N. C. Bray: "Counter-gradient diffusion in premixed turbulent flames". AIAA J. 19, 205-213 (1981).
2. I. G. Shepherd, J. B. Moss, K. N. C. Bray; "Turbulent transport in a confined premixed flame". Nineteenth Symp. (International) on Combustion, p. 423, The Combustion Inst. (1982).
3. I. G. Shepherd, J. B. Moss: "Characteristic scales for density fluctuations in a turbulent premixed flame". Combust. Sci. and Tech. 33, 231-243 (1983).
4. K. N. C. Bray, P. A. Libby, G. Masuya, J. B. Moss: "Turbulence production in premixed turbulent flames". Combust. Sci. and Tech. 25, 127 (1981).
5. K. N. C. Bray, P. A. Libby, J. B. Moss: "Flamelet crossing frequencies and mean reaction rates in premixed turbulent combustion". Combust. Sci. and Tech. 41, 143-172 (1984).
6. F. C. Gouldin, R. N. Halthore: "Rayleigh scattering for density measurements in premixed flames". Experiments in Fluids, to appear (1986).
7. M. Namazian, I. G. Shepherd, L. Talbot: "Characterisation of the density fluctuations in turbulent V-shaped premixed flames". Combust. and Flame 64, 299-308 (1986).
8. K. N. C. Bray: "Methods of including realistic chemical reaction mechanisms in turbulent combustion models". Paper to be presented at Second Workshop on Modelling of Chemical Reaction Systems, Heidelberg, August (1986). To be published.
9. K. N. C. Bray, P. A. Libby, J. B. Moss: "Scalar length scale variations in premixed turbulent flames". Twentieth Symp. (International) on Combustion, pp.421-427, Combustion Inst. (1984).
10. K. N. C. Bray, P. A. Libby, J. B. Moss: "Unified modelling approach for premixed turbulent combustion - Part I: General formulation", Combust. and Flame 61, 87-102 (1985).
11. P. A. Libby: Prog. Combust. Energy Sci. 11, 83-96 (1985).
12. M. F. T. de V. Heitor: "Experiments in turbulent reacting flows". Ph.D. thesis, University of London (1985).
13. R. K. Cheng, L. Talbot, F. Robben: "Conditional velocity statistics in premixed CH<sub>4</sub>-Air and C<sub>2</sub>H<sub>6</sub> - Air turbulent flames". Twentieth Symp. (International) on Combustion, pp.453-461, Combustion Inst. (1984).